

Ethylbenzene
100-41-4 | DTXSID3020596

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.18×10^{-10} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 2.92×10^{-1}

Confidence level: 9.09×10^{-1}

Nearest Neighbors from the Training Set

Image not found

1,3,5-Cycloheptatriene

Measured: 9.69×10^{-11}

Predicted: 1.00×10^{-10}

Image not found

Cyclohepta-1,3-diene

Measured: 1.39×10^{-10}

Predicted: 1.35×10^{-10}

Image not found

1,4-Cyclohexadiene

Measured: 1.00×10^{-10}

Predicted: 1.11×10^{-10}

Image not found

2,5-Norbornadiene

Measured: 1.20×10^{-10}

Predicted: 1.20×10^{-10}